THERMODYNAMIC DATABASE OF VLE AND EXCESS ENTHALPY MEASUREMENTS

Table S-1(a-d) – Datasets containing measurement of VLE and excess enthalpy at temperatures 0°C – 100°C for binaries of C_4 - C_6 hydrocarbons and water with:

a. ***iso*-butanol**

b. ***n*-butanol**

c. **acetone**

d. **ethanol**

Table S-1a. *Iso*-Butanol	**Type**	**Temp. (K)**	**Min. butanol conc. (mol%)**	**Reference**
N-Hexane	VLE (Pxy)	298.15	6.02	Guerrero *et al.* (2010)
	VLE (Pz)	298.15	13.2	Rodriguez *et al.* (1993)
	$\underline{H^E}$	298.15	0.47	Brown *et al.* (1969)
	$\underline{H^E}$	318.15	4.0	Brown *et al.* (1969)
	VLE (Pxy)	332.53	2.04	Berro *et al.* (1982)
Water	VLE (Pxy)	308.15	2.1	Lyzlova *et al.* (1979)[1]
	VLE (Pz)	323.15	0.023	Fischer and Gmehling (1994)
	VLE (Txy)	(1 atm)	(azeo. data)	Stockhardt and Hull (1931)
	VLE (Txy)	(1 atm)	(azeo. data)	Ellis and Garbett (1960)
	γ^{∞}	273 - 373		Fenclova *et al.* (2007)
	x_{Bu}^{sol}	273 - 373		Góral *et al.* (2006)

[1] In Russian; data available in DECHEMA (Gmehling and Onken, 1977)

Table S-1b. *N*-Butanol	**Type**	**Temp. (K)**	**Min. butanol conc. (mol%)**	**Reference**
N-Hexane	VLE (Pz)	283.15	1.2	Gracia *et al.* (1992)
	VLE (Pz)	288.15	1.2	Gracia *et al.* (1992)
	VLE (Pz)	293.15	1.2	Gracia *et al.* (1992)
	VLE (Pz)	298.15	1.2	Gracia *et al.* (1992)
	VLE (Pz)	298.15	4.5	Rodriguez *et al.* (1993)
	$\underline{H}^E$	298.15	16.34	Brown *et al.* (1964)
	VLE (Pz)	303.15	1.2	Gracia *et al.* (1992)
	VLE (Pz)	308.15	1.2	Gracia *et al.* (1992)
	$\underline{H}^E$	308.15	9.41	Brown *et al.* (1964)
	VLE (Pz)	313.15	1.2	Gracia *et al.* (1992)
	VLE (Pz)	318.15	1.2	Gracia *et al.* (1992)
	$\underline{H}^E$	318.15	15.81	Brown *et al.* (1964)
	VLE (Pz)	323.15	1.2	Gracia *et al.* (1992)
	VLE (Pxy)	332.53	0.88	Berro *et al.* (1982)
1-Hexene	$\underline{H}^E$	298.15	4.99	Aguilar *et al.* (2012)
	VLE (Pz)	313.15	5.02	Ghellai *et al.* (2013)
	$\underline{H}^E$	313.15	4.99	Aguilar *et al.* (2012)
N-Pentane	$\underline{H}^E$	298.15	4.82	Collins *et al.* (1980)
	VLE ($PTzV$)	303.15	1.06	Ronc and Ratcliff (1976)[1]
	VLE (Pz)	333.15	1.24	McDougal *et al.* (2014)
	VLE (Pz)	393.15[2]	2.64	McDougal *et al.* (2014)

N-Butane	$\underline{H}^E$	298.15	1.11	McFall *et al.* (1981)
	$\underline{H}^E$	298.15	1.35	Sipowska *et al.* (1994)[3]
	VLE ($PTzV$)	318.4	1.048	Kuitunen *et al.* (2008)
	$\underline{H}^E$	323.15	1.35	Sipowska *et al.* (1994)[3]
	VLE (PTz)	333.15	9.69	Deak *et al.* (1995)
	VLE (PTz)	343.15	9.69	Deak *et al.* (1995)
	$\underline{H}^E$	348.15	1.35	Sipowska *et al.* (1994)[3]
	VLE (PTz)	353.15	9.69	Deak *et al.* (1995)
	VLE (PTz)	363.15	9.69	Deak *et al.* (1995)
	VLE ($PTzV$)	364.5	1.128	Dell'Era *et al.* (2007)
Iso-Butane	VLE ($PTzV$)	318.4	1.016	Kuitunen *et al.* (2008)
1-Butene	VLE ($PTzV$)	318.4	1.221	Kuitunen *et al.* (2008)
	VLE ($PTzV$)	364.5	0.964	Kuitunen *et al.* (2008)
Water	VLE (Pxy)	308.15	1.7	Lyzlova *et al.* (1979)[4]
	VLE (Pz)	322.2	0.018	Fischer and Gmehling (1994)
	γ^{∞}	273 - 373		Dohnal *et al.* (2006)
	x_{Bu}^{sol}	273 - 373		Góral *et al.* (2006)
	Azeotrope			Gmehling (2014)

[1] N.B. raw measurements are contained in the Supplementary Information of Ronc and Ratcliff (1976), available on request (for a fee) from the National Research Council of Canada. These are reproduced in Supplementary Material, Table S-2.

[2] 120°C was outside of the search range, 0 – 100°C, but this dataset was included in order to provide full temperature range for pentane

[3] Measurements at 5, 10, 15 MPa; measurements at 5 MPa used. Effect of pressure on gradient $\partial \underline{H}^E / \partial x_1$ small.

[4] In Russian; dataset available in DECHEMA (Gmehling and Onken, 1977)

Table S-1c. Acetone	**Type**	**Temp. (K)**	**Min. acetone conc. (mol%)**	**Reference**
N-Hexane	$\underline{H^E}$	273.15	15	Schafer and Rohr (1960)[1]
	VLE (Pxy)	293.15	9.13	Rall and Schafer (1959)[1]
	$\underline{H^E}$	293.15	6	Schafer and Rohr (1960)[1]
	$\underline{H^E}$	298.15	5.13	Murakami *et al.* (1964)
	VLE (Pxy)	318.15	6.51	Schafer and Rall (1958)[1]
	VLE (Pxy)	338.15	26.8	Maripuri (1971)
1-Hexene	$\underline{H^E}$	298.15	6.25	Gmehling and Meents (1992)
	VLE (Pxy)[2]	323 - 337	6.0	Ogorodnikov *et al.* (1961)[3]
	$\underline{H^E}$	328.18	6.25	Gmehling and Meents (1992)
N-Pentane	$\underline{H^E}$	273.15	15	Schafer and Rohr (1960)[1]
	$\underline{H^E}$	293.15	6	Schafer and Rohr (1960)[1]
	VLE (Pxy)	298.15	7.77	Rall and Schafer (1959)[1]
	VLE (Pxy)	372.7	8.4	Scott W Campbell *et al.* (1987)
N-Butane	VLE ($PTzV$)	330.2	1.28	Kim *et al.* (2004)
	VLE ($PTzV$)	364.5	1.16	Pasanen *et al.* (2006)
Iso-Butane	VLE ($PTzV$)	318.6	1.27	Kim *et al.* (2004)
	VLE ($PTzV$)	364.5	1.01	Pasanen *et al.* (2006)
1-Butene	VLE ($PTzV$)	323.3	1.26	Kim *et al.* (2004)
	VLE ($PTzV$)	364.5	1.05	Pasanen *et al.* (2006)

Water	VLE (Pz)	288.15	2.01	Rhim *et al.* (1974)[4]
	$\underline{H}^E$	293.15	5.6	Belousov and Sokolova (1966)[5]
	VLE (Pz)	298.15	2.01	Rhim *et al.* (1974)[4]
	VLE (Pz)	308.15	2.01	Rhim *et al.* (1974)[4]
	$\underline{H}^E$	308.15	5.2	Belousov and Sokolova (1966)[5]
	VLE (Pz)	318.15	2.01	Rhim *et al.* (1974)[4]
	VLE (Pz)	323.15	2.90	Chaudhry *et al.* (1980)
	$\underline{H}^E$	323.15	5.7	Belousov and Sokolova (1966)[5]
	VLE (Pz)	373.15	0.33	Griswold and Wong (1952)

[1] In German

[2] Constant pressure (1 bara) data, but limited temperature range

[3] In Russian; data available in DDBST (DDBST, 2017)

[4] In Korean

[5] In Russian, data available in DECHEMA (Gmehling and Onken, 1977)

Table S-1d. Ethanol	**Type**	**Temp. (K)**	**Min. ethanol conc. (mol%)**	**Reference**
N-Hexane	VLE (Pz)	298.15	2.5	Hwang and Robinson (1977)
	VLE (Pxy)	298.15	10	Iguchi (1978)[2]
	$\underline{H^E}$	298.15	3.95	Jones and Lu (1966) [1]
	$\underline{H^E}$	298.15	13.94	Brown *et al.* (1964)
	VLE (Pz)	303.15	1.15	Wolff and Goetz (1976)[2]
	$\underline{H^E}$	308.15	7.38	Brown *et al.* (1964)
	VLE (Pz)	313.15	1.15	Wolff and Goetz (1976)[2]
	VLE (Pxy)	313.15	1.55	Sugi and Katayama (1978)[2]
	$\underline{H^E}$	318.15	13.99	Brown *et al.* (1964)
	VLE (Pxy)	323.15	1.07	Pena and Cheda (1970)[2]
	VLE (Pz)	323.15	1.15	Wolff and Goetz (1976)[2]
	VLE (Pz)	333.15	1.15	Wolff and Goetz (1976)[2]
	VLE (Pxy)	333.15	11.9	Lindberg and Tassios (1971)
	VLE (Pz)	343.15	1.15	Wolff and Goetz (1976)[2]
	VLE (Pz)	353.15	1.15	Wolff and Goetz (1976)[2]
1-Hexene	VLE (Pxy)	333.15	14.1	Lindberg and Tassios (1971)
N-Pentane	VLE (Pxy)	273.15	5	Ishii (1935)[3]
	VLE (Pxy)	283.15	5	Ishii (1935)[3]
	VLE (Pxy)	298.15	5	Ishii (1935)[3]
	$\underline{H^E}$	298.15	9.63	Collins *et al.* (1980)
	VLE (Pz)	303.15	2.52	Reimers *et al.* (1992)
	VLE (Pxy)	372.70	6.3	Scott W. Campbell *et al.* (1987)

N-Butane	VLE (Pxy)	293.15	12.3	Dahlhoff *et al.* (2000)
	$\underline{H}^E$	298.15	1.72	McFall *et al.* (1981)
	$\underline{H}^E$	298.15	2.81	Sipowska *et al.* (1995)
	VLE (Pz)	298.45	5.16	Holderbaum *et al.* (1991)
	VLE (Pxy)	313.2	2.83	Machida *et al.* (2014)
	VLE ($PTzV$)	323.15	0.84	Moilanen *et al.* (2008)
	VLE (PTz)	323.15	10.26	Deak *et al.* (1995)
	$\underline{H}^E$	323.15	1.70	Sipowska *et al.* (1995)
	VLE (Pxy)	323.25	2.56	Soo *et al.* (2009)
	VLE (Pz)	323.75	5.86	Holderbaum *et al.* (1991)
	VLE (PTz)	333.15	10.26	Deak *et al.* (1995)
	VLE (Pxy)	333.2	3.03	Machida *et al.* (2014)
	VLE (PTz)	343.15	10.26	Deak *et al.* (1995)
	VLE (PTz)	345.65	10.26	Deak *et al.* (1995)
	VLE (Pz)	345.65	4.86	Holderbaum *et al.* (1991)
	$\underline{H}^E$	348.15	2.81	Sipowska *et al.* (1995)
	VLE (PTz)	353.15	10.26	Deak *et al.* (1995)
	VLE (Pxy)	353.26	3.78	Soo *et al.* (2009)
	VLE (Pxy)	353.2	8.47	Machida *et al.* (2014)
	VLE (PTz)	363.15	10.26	Deak *et al.* (1995)
	VLE (Pxy)	373.2	10.81	Machida *et al.* (2014)
	VLE (Pxy)	373.27	2.42	Soo *et al.* (2009)

Iso-Butane	VLE (Pxy)	308.6	0.36	Zabaloy *et al.* (1994)
	VLE ($PTzV$)	313.15	0.93	Ouni *et al.* (2005)
	VLE (Pxy)	313.2	9.64	Machida *et al.* (2014)
	VLE (Pxy)	318.4	0.56	Zabaloy *et al.* (1994)
	VLE (Pxy)	333.2	14.70	Machida *et al.* (2014)
	VLE (Pxy)	353.2	15.17	Machida *et al.* (2014)
	VLE (Pxy)	363.5	1.10	Zabaloy *et al.* (1994)
	VLE (Pxy)	373.2	31.14	Machida *et al.* (2014)
1-Butene	VLE ($PTzV$)	326.15	1.01	Laakkonen *et al.* (2003)
Water	VLE, $\underline{H}^E$	273 - 373	-	Voutsas *et al.* (2011)
	γ^∞	273 - 373	-	Dohnal *et al.* (2006)

[1] Results as per chart in paper used; anomalous results from table ignored

[2] Available in DECHEMA (Gmehling and Onken, 1977)

[3] In Japanese; 283.15 & 293.15 K available in DDBST (2017); 273.15 K available in Goral and Oracz (2016)

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SUPPLEMENTARY DATA FROM RONC AND RATCLIFF (1976)

Table S-2 – Supplementary Data Table from Ronc and Ratcliff, for measured $P - z$

z_{Bu}	z_{Pent}	Measured Temperature	Measured Pressure	Pressure at 30°C (Ronc & Ratcliff adjustment[1])
mol/mol	*mol/mol*	*°C*	*bara*[2]	*bara*[2]
0.0000	1.0000	29.982	0.82020	0.82071
0.0106	0.9894	29.993	0.81704	0.81725
0.0336	0.9664	29.987	0.81192	0.81229
0.0755	0.9245	29.988	0.80424	0.80460
0.1226	0.8774	29.980[3]	0.79584	0.79645
0.1810	0.8190	29.984	0.78543	0.78594
0.2284	0.7716	29.978	0.77666	0.77738
0.2785	0.7215	29.982	0.76735	0.76795
0.3339	0.6661	29.983	0.75631	0.75688
0.3799	0.6201	29.983	0.74586	0.74645
0.4292	0.5708	29.990	0.73326	0.73361[4]
0.4735	0.5265	29.983	0.72022	0.72082
0.5095	0.4905	29.978	0.70748	0.70826
0.5341	0.4659	29.985	0.69781	0.69834
0.5576	0.4424	29.977	0.68725	0.68808
0.5585	0.4415	29.982	0.68728	0.68792
0.5808	0.4192	29.979	0.67593	0.67669
0.5942	0.4058	29.980	0.66911	0.66981
0.5949	0.4051	29.980	0.66835	0.66905
0.6332	0.3668	29.978	0.64549	0.64627
0.6752	0.3248	29.984	0.61491	0.61546
0.7186	0.2814	29.978	0.57625	0.57698
0.7609	0.2391	29.979	0.52973	0.53038
0.7945	0.2055	29.978	0.48545	0.48609
0.8170	0.1830	29.977	0.45159	0.45222
0.8497	0.1503	29.984	0.39754	0.39793
0.8823	0.1177	29.980	0.33271	0.33312
0.9206	0.0794	29.982	0.24445	0.24473
0.9503	0.0497	29.978	0.16747	0.16771
0.9636	0.0364	29.976	0.12946	0.12966
0.9801	0.0199	29.982	0.08055	0.08065
0.9923	0.0077	29.981	0.04117	0.04122
0.9963	0.0037	29.976	0.02394	0.02398
1.0000	0.0000	29.993	0.01276	0.01276

[1] Pressure adjustment based on Clausius-Clapeyron to adjust measured pressure to a saturation pressure at an isothermal 30°C (303.15 K):

$$P^{sat}(30^oC) = P^{sat}(T).e^{\frac{\Delta H^{vap}}{R}\left(\frac{1}{T}-\frac{1}{303.15\,K}\right)} \quad \text{(S-1)}$$

The pressure corrections presented in Table S-2, as calculated by Ronc and Ratcliff (1976), were replicated successfully using this formula, save for two anomalies which were explained as minor typos (see [3,4]), assuming ΔH^{vap} was calculated as follows:

$$\Delta H^{vap} = z_{Pent}\Delta H^{vap}_{Pent} + z_{Bu}\,\Delta H^{vap}_{Bu} \quad \text{(S-2)}$$

Where ΔH^{vap}_{Pent} = 26.5 kJ/mol and ΔH^{vap}_{Bu} = 50.2 kJ/mol; *c.f.* DIPPR literature values ΔH^{vap}_{Pent} = 26.1 kJ/mol and ΔH^{vap}_{Bu}= 53.0 kJ/mol (Rowley *et al.*, 2008).

[2] Presented in mmHg (5 s.f.) in original table, conversion of 750.06 mmHg/bara assumed.

[3] In original table, 29.9**9**0, assumed typo for 29.9**8**0 based on analysis of pressure adjustment.

[4] In original table, 550.**52** mmHg, assumed transposition typo for 550.**25** mmHg based on analysis of pressure adjustment.

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PURE COMPONENT PROPERTIES

Table S-3 details the molar masses, critical properties, acentricity and dipole moments of relevant compounds.

Table S-3 – Molar masses, critical properties, acentricity and dipole moments of relevant compounds

Species	Molar Mass	Critical Temperature	Critical Pressure	Critical Molar Volume	Acentric Factor	Dipole Moment	Source
	M_r	T_c	P_c	V_c	ω	μ	
	kg/kmol	*K*	*bara*	$m^3/kmol$	-	*Deybe*	
N-butanol	74.1216	563.10	44.14	0.273	0.58828	1.670	DIPPR
Iso-butanol	74.1216	547.78	43.00	0.273	0.590	1.7	Poling
Ethanol	46.0684	514.00	61.37	0.168	0.64356	1.691	DIPPR
Acetone	58.0791	508.20	47.01	0.209	0.30653	2.881	DIPPR
Water	18.0153	647.10	220.64	0.05595	0.34486	1.850	DIPPR
N-hexane	86.1754	507.60	30.25	0.371	0.30126	0	DIPPR
1-Hexene	84.161	504.00	31.43	0.35510	0.281	0.4	Poling
N-pentane	72.1488	469.70	33.70	0.313	0.25151	0	DIPPR
N-butane	58.1222	425.12	37.96	0.255	0.20016	0	DIPPR
Iso-butane	58.1222	407.80	36.40	0.259	0.18352	0.132	DIPPR
1-Butene	56.1063	419.50	40.20	0.241	0.18450	0.339	DIPPR

Table S-4 – Table S-7 details the parameters and equations for calculation of molar volume; liquid heat capacity and enthalpy; enthalpy of vaporisation; and saturation pressure as a function of temperature of relevant compounds respectively. The parameters were taken mostly from DIPPR (Rowley *et al.*, 2008); where these were not available, from Poling *et al.* (2001); and finally from NIST (2016) where the compound was not available from either.

Throughout, temperature (T) is in Kelvin.

Table S-4 – Parameters for calculation of molar volume as a function of temperature of relevant compounds

Species	A	B	C	D	E	Equation	T_{min}	T_{max}	$\underline{V}^L(T_{min})$	$\underline{V}^L(T_{max})$	Uncertainty
						-	K	K	$kmol/m^3$	$kmol/m^3$	$< \%$
N-butanol	0.98279	0.2683	563.1	0.25488		DIPPR 105	183.85	563.10	12.035	3.663	1
Iso-butanol	10.7631					Fixed (Poling)	273.15	373.15	10.763	10.763	
Ethanol	1.6288	0.27469	514.0	0.23178		DIPPR 105	159.05	514.00	19.410	5.930	1
Acetone	1.2332	0.25886	508.2	0.2913		DIPPR 105	178.45	508.20	15.683	4.764	1
Water	17.863	58.606	-95.396	213.89	-141.26	DIPPR 116	273.16	647.10	55.658	17.863	0.2
N-hexane	0.70824	0.26411	507.6	0.27537		DIPPR 105	177.83	507.60	8.747	2.682	1
1-Hexene	7.9428					Fixed (Poling)	273.15	373.15	7.943	7.943	
N-pentane	0.84947	0.26726	469.7	0.27789		DIPPR 105	143.42	469.70	10.474	3.178	1
N-butane	1.0677	0.27188	425.12	0.28688		DIPPR 105	134.86	425.12	12.620	3.927	1
Iso-butane	1.0631	0.27506	407.8	0.2758		DIPPR 105	113.54	407.80	12.574	3.865	1
1-Butene	1.0877	0.26454	419.5	0.2843		DIPPR 105	87.80	419.50	14.264	4.112	1

DIPPR Equation 105 $$\underline{V}^L(T)[\mathrm{kmol/m^3}] = \frac{A}{B^{1+\left(1-\frac{T}{C}\right)^D}} \quad \text{(S-3)}$$

DIPPR Equation 116 $$\underline{V}^L(T)[\mathrm{kmol/m^3}] = A + B\tau^{0.35} + C\tau^{2/3} + D\tau + E\tau^{4/3} \quad \text{where} \quad \tau = \left(\frac{T}{T_c}\right) \quad \text{(S-4)}$$

Fixed $$\underline{V}^L(T)[\mathrm{kmol/m^3}] = A \quad \text{(S-5)}$$

Table S-5 – Parameters for calculation of liquid heat capacity and enthalpy (relative to temperature $T_0 = 298.15$ K) as a function of temperature of relevant compounds at 1 bara

Species	A	B	C	D	E	Equation	T_{min}	T_{max}	$C_p^L(T_{min})$	$C_p^L(T_{max})$	Uncertainty
	J/kmol/K	*J/kmol/K²*	*J/kmol/K³*	*J/kmol/K⁴*	*J/kmol/K⁵*	-	*K*	*K*	*J/kmol/K*	*J/kmol/K*	*< %*
N-butanol	191200	-730.4	2.2998			DIPPR 100	183.85	391.00	134651	257209	3
Iso-butanol	183000					Fixed	273.15	373.15	183000	183000	
Ethanol	102640	-139.63	-0.0303	0.00204		DIPPR 100	159.05	390.00	87867	164500	3
Acetone	135600	-177	0.2837	0.00069		DIPPR 100	178.45	329.44	116960	132710	1
Water	276370	-2090.1	8.125	-0.0141	9.3701×10^{-6}	DIPPR 100	273.16	533.15	76150	89394	1
N-hexane	172120	-183.78	0.88734			DIPPR 100	177.83	460.00	167500	275340	1
1-Hexene	183300					Fixed (Poling)	273.15	373.15	183000	183000	
N-pentane	159080	-270.5	0.99537			DIPPR 100	143.42	390.00	140760	204980	1
N-butane	191030	-1675	12.5	-0.0387	4.6121×10^{-5}	DIPPR 100	134.86	400.00	112720	222370	1
Iso-butane	172370	-1783.9	14.759	-0.0479	5.805×10^{-5}	DIPPR 100	113.54	380.00	99613	207250	3
1-Butene	182050	-1611	11.963	-0.0375	4.5027×10^{-5}	DIPPR 100	87.80	380.00	110151	181025	1

DIPPR Equation 100

$$C_p^L(T)[\text{J/kmol/K}] = A + BT + CT^2 + DT^3 + ET^4 \quad \text{(S-6)}$$

$$\underline{H}^L(T)[\text{J/kmol}] = A(T - T_0) + \frac{B}{2}(T^2 - T_0^2) + \frac{C}{3}(T^3 - T_0^3) + \frac{D}{4}(T^4 - T_0^4) + \frac{E}{5}(T^5 - T_0^5) \quad \text{(S-7)}$$

Fixed

$$C_p^L(T)[\text{J/kmol/K}] = A \quad \text{(S-8)}$$

$$\underline{H}^L(T)[\text{J/kmol}] = A(T - T_0) \quad \text{(S-9)}$$

Table S-6 – Parameters for calculation of enthalpy of vaporisation as a function of temperature of relevant compounds

Species	A	B	C	D	Equation	T_{min}	T_{max}	$\Delta\underline{H}^{vap}(T_{min})$	$\Delta\underline{H}^{vap}(T_{max})$	Uncertainty
	MJ/kmol				-	*K*	*K*	*MJ/kmol*	*MJ/kmol*	*< %*
N-butanol	71.274	0.0483	0.8966	-0.5116	DIPPR 106	183.85	563.10	63.643	0	3
Iso-butanol	49.100	-1.6587	1.1038	547.7	NIST	298.00	381.00			
Ethanol	65.831	1.1905	-1.7666	1.0012	DIPPR 106	159.05	514.00	50.060	0	1
Acetone	49.258	1.0809	-1.3684	0.69723	DIPPR 106	178.45	508.20	36.605	0	3
Water	56.600	0.61204	-0.6257	0.3988	DIPPR 106	273.16	647.10	44.981	0	1
N-hexane	43.848	0.34057	0.06328	-0.017	DIPPR 106	177.83	507.60	37.532	0	3
1-Hexene	30.400				Fixed (NIST)	273.15	373.15	30.400	30400000	
N-pentane	45.087	0.95886	-0.9238	0.39393	DIPPR 106	143.42	469.70	34.766	0	1
N-butane	36.238	0.8337	-0.8227	0.39613	DIPPR 106	134.86	425.12	28.684	0	3
Iso-butane	39.654	1.274	-1.4255	0.60708	DIPPR 106	113.54	407.80	29.330	0	3
1-Butene	33.774	0.5107	-0.173	0.05181	DIPPR 106	87.80	419.50	30.197	0	3

DIPPR Equation 106 $$\Delta\underline{H}^{vap}(T)[\text{J/kmol}] = A(1-T_r)^{(B+C(T_r)+D(T_r)^2+E(T_r)^3)} \quad \text{(S-10)}$$

NIST $$\Delta\underline{H}^{vap}(T)[\text{J/kmol}] = A.\exp\left(-\frac{BT}{D}\right).\left(1-\frac{T}{D}\right)^{C}$$ where $$T_r = \left(\frac{T}{T_c}\right) \quad \text{(S-11)}$$

Fixed $$\Delta\underline{H}^{vap}(T)[\text{J/kmol}] = A \quad \text{(S-12)}$$

Table S-7 – Parameters for calculation of vapour pressure as a function of temperature of relevant compounds

Species	A	B	C	D	E	$F-I$	Equation	T_{min}	T_{max}	$P^{sat}(T_{max})$	Uncertainty
							-	K	K	$bara$	$<\%$
N-butanol	106.295	-9866.4	-11.655	1.08318×10^{-17}	6		DIPPR 101	183.85	563.10	44.140	3
Iso-butanol	547.78	-8.3146	2.13678	-8.4832	-0.7977	43.04	Poling 3	270.00	547.78	43.040	
Ethanol	73.304	-7122.3	-7.1424	2.8853×10^{-6}	2		DIPPR 101	159.05	514.00	61.086	1
Acetone	69.006	-5599.6	-7.0985	6.2237×10^{-6}	2		DIPPR 101	178.45	508.20	47.091	3
Water	73.649	-7258.2	-7.3037	4.1653×10^{-6}	2		DIPPR 101	289.81	591.95	219.311	0.2
N-hexane	104.65	-6995.5	-12.702	1.2381×10^{-5}	2		DIPPR 101	270.00	624.00	30.449	3
1-Hexene	3.9826	1148.62	225.34	504.03	72	$F = 2.4592$ $G = 106.26$ $H = -3773.6$ $I = 358.15$	Poling 1-2	273.16	647.10	26.860	
N-pentane	78.741	-5420.3	-8.8253	9.6171×10^{-6}	2		DIPPR 101	177.83	507.60	33.642	3
N-butane	66.343	-4363.2	-7.046	9.4509×10^{-6}	2		DIPPR 101	249.98	493.15	37.699	3
Iso-butane	108.43	-5039.9	-15.012	0.02273	1		DIPPR 101	143.42	469.70	36.299	1
1-Butene	51.836	-4019.2	-4.5229	4.8833×10^{-17}	6		DIPPR 101	134.86	425.12	40.213	3

DIPPR Equation 101 $$P^{vap}(T)[\text{Pa}] = \exp\left(A + \frac{B}{T} + C.\ln T + DT^{E}\right) \quad \text{(S-1)}$$

Poling 1-2 Equation $$P^{vap}(T)[\text{Pa}] = \begin{cases} 10^{\left(5+A-\frac{B}{(T+C-273.15)}\right)}, & T < I \\ 10^{\left(5+A-\frac{B}{(T+C-273.15)}+0.43429X^{F}+GX^{8}+HX^{12}\right)}, & T \geq I \end{cases} \quad \text{where} \quad X = \frac{T-E-273.15}{D} \quad \text{(S-2)}$$

Poling 3 Equation $$P^{vap}(T)[\text{Pa}] = (10^{5})\exp\left(\ln F + \left(\frac{A}{T}\right)(B\tau + C\tau^{1.5} + D\tau^{2.5} + E\tau^{5})\right) \quad \text{where} \quad \tau = 1 - \frac{T}{A} \quad \text{(S-3)}$$

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LEGENDRE ACTIVITY MODEL COEFFICIENTS FOR FERMENTATION PRODUCTS WITH SELECT $C_4 - C_6$ HYDROCARBONS AND WATER

Table S-8a-t – Temperature-dependant Legendre activity model coefficients determined for *n*-butanol, *iso*-butanol, ethanol and acetone with $C_4 - C_6$ hydrocarbons and water, regressed using the virial equation of state ($T_{ref} = 298.15\ K$)

a. ***n*-Butanol (1)/*n*-hexane (2)**

Legendre Coefficient k	a_k	b_k	c_k
$k = 0$	1.9942	1.0414	8.5104
$k = 1$	-0.5886	-0.6852	-9.7109
$k = 2$	0.3886	0.6086	6.4714
$k = 3$	-0.1728	-0.0804	-8.3159
$k = 4$	0.0920	0.2842	3.8338
$k = 5$	-0.0217	0.0095	-3.7914

b. ***n*-Butanol (1)/1-hexene (2)**

Legendre Coefficient k	a_k	b_k	c_k
$k = 0$	1.8194	1.0646	9.8553
$k = 1$	-0.5344	-0.9350	-8.9473
$k = 2$	0.2216	0.2541	8.9390
$k = 3$	-0.0850	0.0194	-7.5451

c. ***n*-Butanol (1)/*n*-pentane (2)**

Legendre Coefficient k	a_k	b_k	c_k
$k = 0$	1.9091	0.9377	9.1357
$k = 1$	-0.6270	-0.9187	-3.8084
$k = 2$	0.3185	0.5959	3.3896
$k = 3$	-0.1431	-0.3626	-0.4391
$k = 4$	0.0440	0.1941	0.5930

d. ***n*-Butanol (1)/*iso*-butane (2)**

Legendre Coefficient k	a_k	b_k	c_k
$k = 0$	1.8371	0.0000	0.0000
$k = 1$	-0.6336	0.0000	0.0000
$k = 2$	0.3334	0.0000	0.0000
$k = 3$	-0.1822	0.0000	0.0000
$k = 4$	0.1029	0.0000	0.0000
$k = 5$	-0.0413	0.0000	0.0000
$k = 6$	0.0205	0.0000	0.0000
$k = 7$	-0.0008	0.0000	0.0000

e. ***n*-Butanol (1)/*n*-butane (2)**

Legendre Coefficient k	a_k	b_k	c_k
$k = 0$	1.8342	0.7476	7.5606
$k = 1$	-0.6569	-0.8318	-6.7276
$k = 2$	0.3065	0.5045	4.7080
$k = 3$	-0.1221	-0.2165	-2.6630

f. ***n*-Butanol (1)/1-butene (2)**

Legendre Coefficient *k*	a_k	b_k	c_k
$k = 0$	1.7469	2.1107	0.0000
$k = 1$	-0.7192	-2.0156	0.0000
$k = 2$	0.3614	1.3434	0.0000
$k = 3$	-0.2069	-0.9319	0.0000
$k = 4$	0.1180	0.6303	0.0000
$k = 5$	-0.0582	-0.3297	0.0000
$k = 6$	0.0298	0.1987	0.0000
$k = 7$	-0.0090	-0.0541	0.0000
$k = 8$	0.0043	0.0339	0.0000
$k = 9$	0.0003	0.0063	0.0000

g. **Acetone (1)/*n*-hexane (2)**

Legendre Coefficient *k*	a_k	b_k	c_k
$k = 0$	1.8019	2.7323	1.1910
$k = 1$	0.0738	-0.3222	-1.9821
$k = 2$	0.0697	0.3531	-2.3365
$k = 3$	0.0301	0.0038	-0.6567

h. **Acetone (1)/1-hexene (2)**

Legendre Coefficient *k*	a_k	b_k	c_k
$k = 0$	2.2680	1.9265	0.8439
$k = 1$	0.0307	-0.1020	0.3267
$k = 2$	-0.3008	0.1083	-0.8086
$k = 3$	-0.2926	0.0238	0.4050
$k = 4$	-0.0476	0.0015	-0.6490

i. **Acetone (1)/*n*-pentane (2)**

Legendre Coefficient k	a_k	b_k	c_k
$k = 0$	1.8131	2.6537	1.7789
$k = 1$	-0.1385	-0.4049	-1.0666
$k = 2$	0.1934	0.5905	-0.5037
$k = 3$	-0.0492	-0.2361	-1.0770
$k = 4$	0.0292	0.0935	-0.2822

j. **Acetone (1)/*iso*-butane (2)**

Legendre Coefficient k	a_k	b_k	c_k
$k = 0$	1.7005	2.4786	0.0000
$k = 1$	-0.1798	-0.5212	0.0000
$k = 2$	0.1106	0.2310	0.0000
$k = 3$	-0.0269	-0.0481	0.0000
$k = 4$	0.0069	-0.0189	0.0000
$k = 5$	-0.0025	-0.0006	0.0000
$k = 6$	0.0006	0.0000	0.0000

k. **Acetone (1)/*n*-butane (2)**

Legendre Coefficient k	a_k	b_k	c_k
$k = 0$	1.6972	2.4939	0.0000
$k = 1$	-0.1894	-0.4223	0.0000
$k = 2$	0.1217	0.2852	0.0000
$k = 3$	-0.0249	-0.0239	0.0000
$k = 4$	0.0134	0.0437	0.0000
$k = 5$	0.0014	0.0212	0.0000
$k = 6$	0.0038	0.0260	0.0000
$k = 7$	0.0021	0.0118	0.0000

l. **Acetone (1)/1-butene (2)**

Legendre Coefficient k	a_k	b_k	c_k
$k = 0$	1.2205	1.5249	0.0000
$k = 1$	-0.1914	-0.3770	0.0000
$k = 2$	0.0664	0.0847	0.0000
$k = 3$	-0.0170	-0.0044	0.0000
$k = 4$	-0.0002	-0.0418	0.0000
$k = 5$	0.0001	0.0145	0.0000
$k = 6$	-0.0013	-0.0100	0.0000

m. **Ethanol (1)/*n*-hexane (2)**

Legendre Coefficient k	a_k	b_k	c_k
$k = 0$	2.4371	1.1518	7.1185
$k = 1$	-0.3591	-0.6494	-4.6249
$k = 2$	0.4471	0.6210	3.7075
$k = 3$	-0.1360	-0.3056	-1.1105
$k = 4$	0.0921	-0.0106	3.4309

n. **Ethanol (1)/1-hexene (2)**

Legendre Coefficient k	a_k	b_k	c_k
$k = 0$	2.1025	0.0000	0.0000
$k = 1$	-2.3572	0.0000	0.0000
$k = 2$	0.9516	0.0000	0.0000
$k = 3$	-2.5705	0.0000	0.0000
$k = 4$	1.1487	0.0000	0.0000
$k = 5$	-1.5429	0.0000	0.0000
$k = 6$	0.5198	0.0000	0.0000
$k = 7$	-0.3465	0.0000	0.0000
$k = 8$	0.0317	0.0000	0.0000
$k = 9$	-0.0000	0.0000	0.0000

o. **Ethanol (1)/*n*-pentane (2)**

Legendre Coefficient k	a_k	b_k	c_k
$k = 0$	2.3309	1.0265	14.3952
$k = 1$	-0.5417	-0.5941	3.8963
$k = 2$	0.3860	0.5503	14.7126
$k = 3$	-0.1776	-0.2668	6.6361
$k = 4$	0.0833	0.1365	7.0649
$k = 5$	-0.0183	-0.0413	5.7851
$k = 6$	0.0195	-0.0036	1.6065

p. **Ethanol (1)/*iso*-butane (2)**

Legendre Coefficient k	a_k	b_k	c_k
$k = 0$	2.3345	2.2748	-0.0490
$k = 1$	-0.5398	-1.3983	0.2734
$k = 2$	0.4404	1.9512	-5.1718
$k = 3$	-0.2449	-2.9677	20.5388
$k = 4$	0.0430	-0.7886	8.7774
$k = 5$	-0.0875	-2.2341	17.8208

q. **Ethanol (1)/*n*-butane (2)**

Legendre Coefficient k	a_k	b_k	c_k
$k = 0$	2.2403	0.8800	7.9894
$k = 1$	-0.5559	-0.6479	-7.8321
$k = 2$	0.3207	0.5425	4.9754
$k = 3$	-0.1229	-0.2483	-2.7241

r. **Ethanol (1)/1-butene (2)**

Legendre Coefficient k	a_k	b_k	c_k
$k = 0$	1.9614	0.0000	0.0000
$k = 1$	-0.4761	0.0000	0.0000
$k = 2$	0.2620	0.0000	0.0000
$k = 3$	-0.1217	0.0000	0.0000
$k = 4$	0.0522	0.0000	0.0000
$k = 5$	-0.0205	0.0000	0.0000
$k = 6$	0.0014	0.0000	0.0000

s. ***iso*-Butanol (1)/*n*-hexane (2)**

Legendre Coefficient k	a_k	b_k	c_k
$k = 0$	1.9463	1.3950	6.5765
$k = 1$	-0.5536	-0.9648	-11.6639
$k = 2$	0.2826	0.8904	-1.6218
$k = 3$	-0.1132	-0.0128	-16.4772

t. **Acetone (1)/Water (2)**

Legendre Coefficient k	a_k	b_k	c_k
$k = 0$	1.82252	-0.45830	7.31812
$k = 1$	-0.04096	2.28855	-2.10511
$k = 2$	0.07353	-0.37220	2.00220
$k = 3$	-0.01546	0.50351	0.21347
$k = 4$	-0.00970	0.00596	-0.79401